

Score-based Generative Modeling of Graphs via the System of Stochastic Differential Equations

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Abstract

Generating graph-structured data requires learning the underlying distribution of graphs. Yet, this is a challenging problem, and the previous graph generative methods either fail to capture the permutation-invariance property of graphs or cannot sufficiently model the complex dependency between nodes and edges, which is crucial for generating real-world graphs such as molecules. To overcome such limitations, we propose a novel score-based generative model for graphs with a continuous-time framework. Specifically, we propose a new graph diffusion process that models the joint distribution of the nodes and edges through a system of stochastic differential equations (SDEs). Then, we derive novel score matching objectives tailored for the proposed diffusion process to estimate the gradient of the joint log-density with respect to each component, and introduce a new solver for the system of SDEs to efficiently sample from the reverse diffusion process. We validate our graph generation method on diverse datasets, on which it either achieves significantly superior or competitive performance to the baselines. Further analysis shows that our method is able to generate molecules that lie close to the training distribution yet do not violate the chemical valency rule, demonstrating the effectiveness of the system of SDEs in modeling the node-edge relationships. Our code is available at <https://github.com/harryjo97/GDSS>.